

# High-order fidelity and quantum phase transition for the Heisenberg chain with next-nearest-neighbor interaction

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In this article, we study the high order term of the fidelity of the Heisenberg chain with next-nearest-neighbor interaction and analyze its connection with quantum phase transition of Beresinskii-Kosterlitz-Thouless type happened in the system. We calculate the fidelity susceptibility of the system and find that although the phase transition point can't be well characterized by the fidelity susceptibility, it can be effectively picked out by the higher order of the ground-state fidelity for finite-size systems.

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## I. INTRODUCTION

Quantum phase transitions (QPTs) of a quantum many-body system have been attracting the persistent interest of physical researchers in recent years. Due to the diversity of quantum phases and QPTs, finding universal ways or methods to characterize QPTs is very meaningful and urgent. From the viewpoint of Landau-Ginzburg theory which has been widely accepted and known in condensed matter physics [1], QPT is connected with the corresponding order parameter and symmetry breaking. However, there are also some QPTs which cannot be well understood under the Landau-Ginzburg paradigm, such as the topological phase transitions [2] and Beresinskii-Kosterlitz-Thouless (BKT) phase transitions [3, 4]. Recently, an increasing research effort has been focused on the role of ground-state fidelity in characterizing QPTs [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. As a basic concept in quantum information science, the fidelity measures the similarity between two states and is simply defined as modulus of their overlap [7]. The fidelity approach provides us a novel way to understand QPTs from the viewpoint of quantum information theory. So far QPTs in various quantum many-body systems [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] have been shown to be well characterized by the ground-state fidelity or fidelity susceptibility which is the leading term of the fidelity [13, 14].

Generally, one may expect that the structure of the ground states at the different phases is basically different and should reveal itself by some sort of singular behavior in the ground state fidelity or the fidelity susceptibility at the transition point [7, 8]. Despite its great successes of application in various systems, this intuitive idea turns out to be not complete [10, 11, 12, 13, 16]. Although the fidelity and the fidelity susceptibility can be used to describe first- and second-order QPTs [11], as well as the

topological QPTs [19, 20, 21, 22] successfully, nevertheless there are also some ambiguous cases for that both the two methods mentioned above do not work very effectively [10, 11, 13, 16]. Very recently, the controversial issue of BKT phase transition and ground state fidelity has been studied in Ref. [17] from a perspective of matrix product states which essentially depend on a classical simulations of quantum lattice systems [15].

In case that the leading term of the fidelity (fidelity susceptibility) works not very effectively, the higher order term in the fidelity may be worth studying. Up to now, there is still lack of literature concerning this part of the fidelity. Here, in this paper, we make an attempt on investigating the effect of higher order term of the fidelity on the characterization of the BKT-type phase transition happened in the Heisenberg chain with next-nearest-neighbor (NNN) interaction [27]. We will show that although the fidelity and fidelity susceptibility cannot effectively characterize the BKT-type phase transition point for the Heisenberg chain with NNN interaction, the higher order term of the fidelity gives a good attempt on detecting such a transition.

Our paper is organized as follows. In Sec. II, we display the formulism of the higher order term of the fidelity. The subsequent section is devoted to the calculation of the higher order term of the fidelity for the model of Heisenberg chain with NNN interaction and show its connection to the quantum phase transition of the system. A brief summary is given in Sec. IV.

## II. HIGHER ORDER OF THE FIDELITY

As usual, the ground state fidelity is defined as the modulus of the overlap between  $|\Psi_0(\lambda)\rangle$  and  $|\Psi_0(\lambda+\delta\lambda)\rangle$ , i.e.

$$F(\lambda, \delta\lambda) = |f(\lambda, \lambda + \delta\lambda)| = |\langle \Psi_0(\lambda) | \Psi_0(\lambda + \delta\lambda) \rangle|, \quad (1)$$

where  $\Psi_0(\lambda)$  is the ground-state wavefunction of Hamiltonian  $H = H_0 + \lambda H_I$ ,  $\lambda$  is the driving parameter and  $\delta\lambda$

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is a small deviation in the parameter space of  $\lambda$ . The fidelity susceptibility denotes only the leading term of the fidelity. Straightforwardly, one can get the higher order term of the fidelity following similar expansion in deriving the fidelity susceptibility [13]. By using the Taylor expansion, the overlap between two wavefunction  $|\Psi_0(\lambda)\rangle$  and  $|\Psi_0(\lambda + \delta\lambda)\rangle$  can be expanded to an arbitrary order of  $\delta\lambda$ , i.e.

$$f(\lambda, \lambda + \delta\lambda) = 1 + \sum_{n=1}^{\infty} \frac{(\delta\lambda)^n}{n!} \left\langle \Psi_0(\lambda) \left| \frac{\partial^n}{\partial \lambda^n} \Psi_0(\lambda) \right. \right\rangle. \quad (2)$$

Therefore, the fidelity becomes

$$\begin{aligned} F^2 = & 1 + \sum_{n=1}^{\infty} \frac{(\delta\lambda)^n}{n!} \left\langle \Psi_0 \left| \frac{\partial^n}{\partial \lambda^n} \Psi_0 \right. \right\rangle + \\ & \sum_{n=1}^{\infty} \frac{(\delta\lambda)^n}{n!} \left\langle \frac{\partial^n}{\partial \lambda^n} \Psi_0 \left| \Psi_0 \right. \right\rangle + \\ & \sum_{m,n=1}^{\infty} \frac{(\delta\lambda)^{m+n}}{m!n!} \left\langle \Psi_0 \left| \frac{\partial^n}{\partial \lambda^n} \Psi_0 \right. \right\rangle \left\langle \frac{\partial^m}{\partial \lambda^m} \Psi_0 \left| \Psi_0 \right. \right\rangle. \end{aligned} \quad (3)$$

We note that  $\frac{\partial^n}{\partial \lambda^n} \langle \Psi_0(\lambda) | \Psi_0(\lambda) \rangle = 0$  and use the relation for a given  $n$

$$\sum_{m=0}^n \frac{n!}{m!(n-m)!} \left\langle \frac{\partial^m}{\partial \lambda^m} \Psi_0 \left| \frac{\partial^{n-m}}{\partial \lambda^{n-m}} \Psi_0 \right. \right\rangle = 0, \quad (4)$$

then we can simplify the expression of (3) into

$$F^2 = 1 - \sum_{l=1}^{\infty} (\delta\lambda)^l \chi_F^{(l)} \quad (5)$$

where

$$\chi_F^{(l)} = \sum_{l=m+n} \frac{1}{m!n!} \left\langle \frac{\partial^m}{\partial \lambda^m} \Psi_0 \left| \hat{P} \left| \frac{\partial^n}{\partial \lambda^n} \Psi_0 \right. \right. \right\rangle, \quad (6)$$

with the projection operator  $\hat{P}$  defined as  $\hat{P} = 1 - |\Psi_0\rangle\langle\Psi_0|$ . It is easy to check that  $\chi_F^{(1)}$  is zero and  $\chi_F^{(2)}$  the fidelity susceptibility [13].

Next we shall consider the third order fidelity  $\chi_F^{(3)}$  and apply it to judge the phase transition in the spin chain model with NNN exchanges. Alternatively, one can directly derive the expression of  $\chi_F^{(3)}$  from the perturbation expansion of the GS wavefunction. According the perturbation theory, the GS wavefunction, up to the second

order, is

$$\begin{aligned} |\Psi_0(\lambda + \delta\lambda)\rangle = & |\Psi_0\rangle + \delta\lambda \sum_{n \neq 0} \frac{H_I^{n0} |\Psi_n\rangle}{E_0 - E_n} \\ & + (\delta\lambda)^2 \sum_{m,n \neq 0} \frac{H_I^{nm} H_I^{m0} |\Psi_n\rangle}{(E_0 - E_m)(E_0 - E_n)} \\ & - (\delta\lambda)^2 \sum_{n \neq 0} \frac{H_I^{00} H_I^{n0} |\Psi_n\rangle}{(E_0 - E_n)^2} \\ & - \frac{(\delta\lambda)^2}{2} \sum_{n \neq 0} \frac{H_I^{0n} H_I^{n0} |\Psi_0\rangle}{(E_0 - E_n)^2}. \end{aligned}$$

The 3rd order term  $\chi_F^{(3)}$ , which is proportional to the 3rd order derivative of GS fidelity, can be then directly extracted from eq. (5):

$$\chi_F^{(3)} = \sum_{m,n \neq 0} \frac{2H_I^{0m} H_I^{mn} H_I^{n0}}{(E_0 - E_m)(E_0 - E_n)^2} - \sum_{n \neq 0} \frac{2H_I^{00} |H_I^{n0}|^2}{(E_0 - E_n)^3}. \quad (8)$$

Eqs. (6) and (8) present the main formulism of the higher order expansion of the fidelity. So far the explicit physical meaning of the high order term in the fidelity is still not clear. The expression of 3rd fidelity bears the similarity to its correspondence of the 3rd derivative of GS energy which has the following form

$$\frac{\partial^3 E}{\partial \lambda^3} = \sum_{m,n \neq 0} \frac{6H_I^{0m} H_I^{mn} H_I^{n0}}{(E_0 - E_m)(E_0 - E_n)} - \sum_{n \neq 0} \frac{6H_I^{00} |H_I^{n0}|^2}{(E_0 - E_n)^2}. \quad (9)$$

Obviously, the 3rd fidelity is more divergent than the 3rd derivative of GS energy. Similar connection between the fidelity susceptibility and 2nd derivative of GS energy has been unveiled [11]. Generally the  $n$ -th order fidelity is much more divergent than its counterpart of  $n$ -th order derivative of GS energy, therefore an  $n$ -th order QPT can be certainly detected by the  $n$ -th order fidelity. However, this conclusion does not exclude the possibility that  $n$ -th order fidelity can detect a even higher order or infinite order QPT. A concrete example has been given in Ref. [16], where a QPT of higher than second order was singled out unambiguously by using the fidelity susceptibility despite the corresponding second derivative of the ground-state energy density showing no signal of divergence. So far no example of BKT-type QPT unambiguously detected by fidelity susceptibility has been given. Next we shall attempt to apply the third-order fidelity to study the BKT-type transition in a the spin chain model with NNN exchanges.

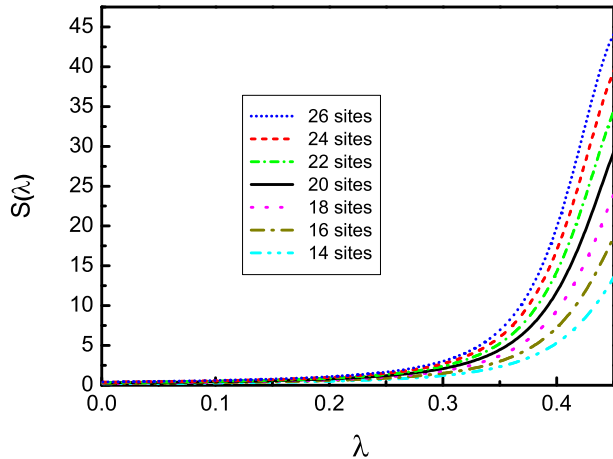


FIG. 1: The GS fidelity susceptibility of the heisenberg chain with next-nearest-neighbor interaction for finite system size from 14 sites to 26 sites. Obviously, there is no expected peaks can be observed.

### III. THE MODEL AND THE CALCULATION OF 3RD ORDER FIDELITY

Now we turn to the one-dimensional Heisenberg chain with the NNN coupling described by the Hamiltonian

$$H(\lambda) = \sum_{j=1}^L (\hat{s}_j \hat{s}_{j+1} + \lambda \hat{s}_j \hat{s}_{j+2}), \quad (10)$$

where  $\hat{s}_j$  denotes the spin-1/2 operator at the  $j$ th site,  $L$  denotes the total number of sites. The driving parameter  $\lambda$  represents the ratio between the NNN coupling and the nearest-neighbor (NN) coupling. The GS properties of the model (10) has been widely studied by both analytical method [27, 30] and numerical method [28, 29, 31, 32]. The QPT driven by  $\lambda$  is well understood. The driving term due to  $\lambda$  is irrelevant when  $\lambda < \lambda_c (\simeq 0.2411)$ , and the system flows to a spin fluid or Luttinger liquid with massless spinon excitations. As  $\lambda > \lambda_c$ , the frustration term is relevant and the ground state flows to the dimerized phase with a spin gap open [27, 30]. The transition from spin fluid to dimerized phase is known to be of BKT type [27, 30], for which the transition point was hard to be determined numerically due to the problem of logarithmic correction [33]. The critical value of  $\lambda_c = 0.2411 \pm 0.0001$  has been accurately determined by various numerical methods [28, 29, 31, 32].

The GS fidelity for the model (10) has been studied in Ref. [10] and also in Ref. [26] in terms of operator fidelity. No singularities in the GS fidelity or operator fidelity around  $\lambda_c$  have been detected for the system with different sizes, which implies that the GS fidelity may be not an effective characterization of the BKT-type QPT in

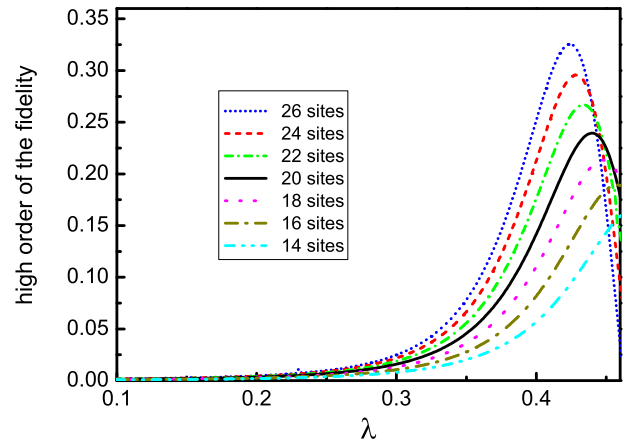


FIG. 2: The third order term of the GS fidelity of the spin chain with next-nearest-neighbor interaction for the finite system size from 14 sites to 26 sites. Explicit peaks can be observed in this figure. As the system size increases, the position of the peak gets closer to the BKT-transition point.

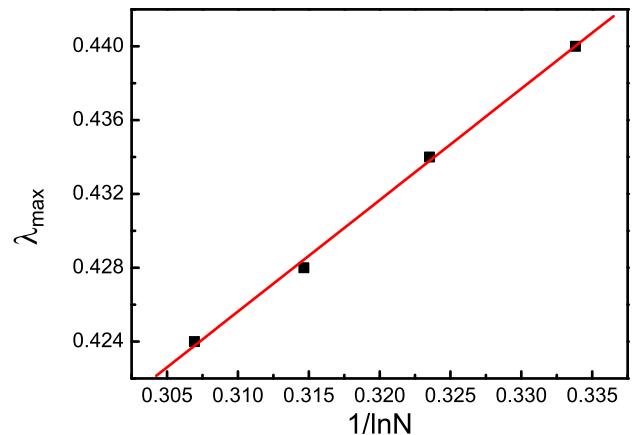


FIG. 3: Finite-size scaling of the extrema of the third term of the GS fidelity. A linear fit is made. According to this fit, when it comes to the point  $N \rightarrow \infty$ ,  $\lambda_c = 0.238 \pm 0.006$ .

this model. The BKT-type QPT is a infinite order phase transition where the  $n$ -th order derivative of GS energy is continuous. In light of the higher-order fidelity being more powerful than its energy judgement, we study the possibility for detecting the infinite-order BKT-type QPT via the 3rd order fidelity and focus on the QPT in the spin chain with NNN interactions as a concrete example. We first calculate the GS wave functions by using the numerical exact diagonalization method for fi-

nite size system, and thus the fidelity susceptibility and the 3rd order fidelity can be extracted from the overlap of neighboring GS wave functions. In Fig.1, we display the fidelity susceptibility for systems with different sizes. We observe that no an obvious peak for the fidelity susceptibility is detected in a wide range of the parameter  $0 < \lambda < 0.5$ . This result suggests that the transition point for the BKT-type QPTs cannot be very effectively characterized by the fidelity susceptibility either for a finite-size system.

The BKT-type phase transition generally is an infinite order phase transition for which the infinite order derivatives of the ground-state energy is continuous. A good example with exact proof is the BKT-type transition happened in the antiferromagnetic XXZ spin chain model [34]. In the BKT-type transition point, it has been proven analytically that all the  $n$ -th order derivatives of ground state energy is continuous [34]. Since the  $n$ -th order fidelity is much divergent than its correspondence of derivative of the ground-state energy, one might expect that there exists the possibility that the  $n$ -th order fidelity is divergent even its  $n$ -th order energy derivative is continuous. To see whether a higher order fidelity works better than fidelity susceptibility in detecting the BKT-type QPT happened in this model, we calculated the 3rd order fidelity versus the driving parameter as shown in Fig. 2. It is clear that a peak is developed in the 3rd order fidelity and the location of peaks tends to get close to the side of transition point  $\lambda_c$  with the increase of lattice size. To extrapolate the  $\lambda_c$  in the infinite size limit, we analyze the finite size scaling of position of peak in the Fig. 3. When the system size comes to infin-

ity, the extrapolated value of the phase transition point is  $\lambda_c = 0.238 \pm 0.006$ , which, within the scope of fitting error, agrees well with  $\lambda_c = 0.2411 \pm 0.0001$  obtained by highly accurate numerical methods [28, 29, 31, 32].

#### IV. SUMMARY

We have shown the formulism for the high order of the fidelity in detail and applied it to a concrete model, *i.e.*, the one dimensional Heisenberg chain with NNN interaction. We first calculate the ground-state wavefunction of the system by exact diagonalization method, and then extract fidelity susceptibility and the third order of the GS fidelity. We find that despite the GS fidelity and the fidelity susceptibility being not a very effective detector, the BKT-type phase transition happened in this spin chain model might be effectively detected by the 3rd order term of the GS fidelity for finite-size system. Although the physical meaning of the higher order term of the GS fidelity hasn't been deeply understood, we wish that our observation would stimulate further studies on this issue.

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